

Tioclorim [ISO]
68925-41-7 | DTXSID30218994

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 234 °C

Global applicability domain: Inside

Local applicability domain index: 3.56e-01

Confidence level: 3.77e-01

Nearest Neighbors from the Training Set

Image not found

Allopurinol

Measured: 350

Predicted: 287

Image not found

1,4-Benzenediamine, N-(2,4-dinitrophenyl)-

Measured: 188

Predicted: 189

Image not found

Anot

Measured: 199

Predicted: 199

Image not found

4-Nitro-1,2-phenylenediamine

Measured: 200

Predicted: 182

Image not found

Brodimoprim

Measured: 227

Predicted: 226